

One Dimensional Regularizations of the Coulomb Potential with Application to Atoms in Strong Magnetic Fields

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ABSTRACT. It is well-known that the functions $V_m(x) = \frac{1}{\Gamma(m+1)} \int_0^\infty \frac{u^m e^{-u}}{\sqrt{x^2+u}} du$ arise naturally in the study of atoms in strong magnetic fields where they can be regarded as one-dimensional regularizations of the Coulomb potential. For many-electron atoms consideration of the Pauli principle requires convex combinations of such potentials and interactions of the form $\frac{1}{\sqrt{2}} V_m(\frac{|x_1-x_2|}{\sqrt{2}})$. We summarize the results of a comprehensive study of these functions including recursion relations, tight bounds, convexity properties, and connections with confluent hypergeometric functions. We also report briefly on their application in one-dimensional models of many-electron atoms in strong magnetic fields.

1. Introduction

It is well-known that systems in strong magnetic fields behave like systems in one-dimension, i.e., a strong magnetic field confines the particles to Landau orbits orthogonal to the field, leaving only their behavior in the direction of the field subject to significant influence by a static potential. Motivated by this general principle and the work of Lieb, Solovej and Yngvason [LSY] on atoms in extremely strong magnetic fields, Brummelhuis and Ruskai [BR1] initiated a study of models of atoms in homogeneous strong magnetic fields in which the 3-dimensional wavefunction has the form

$$(1.1) \quad \Psi(\mathbf{r}_1, \mathbf{r}_2 \dots \mathbf{r}_n) = \psi(x_1 \dots x_n) \Upsilon(y_1, z_1, y_2, z_2, \dots y_n, z_n)$$

where Υ lies in the projection onto the lowest Landau band for an N-electron system. We follow the somewhat non-standard convention of choosing the magnetic field in the x-direction, i.e, $\mathbf{B} = (B, 0, 0)$ where B is a constant denoting the field strength, in order to avoid notational confusion with the nuclear charge Z .

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Such models lead naturally to one dimensional regularizations of the Coulomb potentials of the form

$$(1.2) \quad V_m(x) = \int_0^{2\pi} \int_0^\infty \frac{|\gamma_m(r, \theta)|^2}{\sqrt{x^2 + r^2}} r dr d\theta$$

$$(1.3) \quad = \frac{1}{\Gamma(m+1)} \int_0^\infty \frac{u^m e^{-u}}{\sqrt{x^2 + u}} du$$

$$(1.4) \quad = \frac{2e^{x^2}}{\Gamma(m+1)} \int_{|x|}^\infty (t^2 - x^2)^m e^{-t^2} dt$$

where $\gamma_m(r, \theta) = \frac{1}{\sqrt{\pi m!}} e^{-im\theta} r^m e^{-r^2/2}$. Recognition that such potentials are important goes back at least to Schiff and Snyder [SS] in 1939 and played an important role in the Avron, Herbst and Simon study [AHS] of hydrogen. Recently, Ruskai and Werner [RW] undertook a detailed study of these potentials, proving the important property of convexity of $1/V_m$ as well as a number of other useful properties. The primary purpose of this note is to give a summary of these results in Sections 4 and 5. Before doing that, we briefly discuss one-dimensional models of atoms in strong magnetic fields in Section 2 and their implications for the maximum negative ionization problem in Section 3.

2. Atoms in Strong Magnetic Fields

The Hamiltonian for an N electron atom in a magnetic field \mathbf{B} is

$$(2.1) \quad H(N, Z, B) = \sum_{j=1}^N \left[|\mathbf{P}_j + \mathbf{A}|^2 - \frac{Z}{|\mathbf{r}_j|} \right] + \sum_{j < k} \frac{1}{|\mathbf{r}_j - \mathbf{r}_k|}$$

where \mathbf{A} is a vector potential such that $\nabla \times \mathbf{A} = \mathbf{B}$. The ground-state energy of $H(N, Z, B)$ is given by

$$(2.2) \quad E_0(N, Z, B) = \inf_{\|\Psi\|=1} \langle H(N, Z, B)\Psi, \Psi \rangle$$

Let $E_0^{\text{conf}}(N, Z, B)$ denote the corresponding minimum restricted to functions of the form (1.1). For extremely strong fields, it was shown in [LSY] that $E_0/E_0^{\text{conf}} \rightarrow 1$ as $B/Z^{4/3} \rightarrow \infty$ with N/Z fixed.

In [BR1] and [BR2] we consider two special cases of (1.1). We write the Landau state with angular momentum m in the x -direction in the form

$$(2.3) \quad \gamma_m^B(y, z) = \frac{B^{(m+1)/2}}{\sqrt{\pi m!}} \zeta^m e^{-B|\zeta|^2/2}$$

where $\zeta = y + iz$. Then our two special cases can be described as follows:

Zero model: In this case, we make the extremely simple assumption that Υ is simply a product of Landau states with $m = 0$, i.e., $\Upsilon = \prod_{k=1}^N \gamma_0(y_k, z_k)$.

Slater model: In this case we assume that Υ is an antisymmetrized product of Landau states with $m = 0, 1, \dots, N-1$, i.e., $\Upsilon = \frac{1}{\sqrt{N!}} [\gamma_0 \wedge \gamma_1 \wedge \dots \wedge \gamma_{N-1}]$.

Although the first model is somewhat unrealistic, its simplicity makes it amenable to detailed analysis which yields insight into the general situation. The second model corresponds to the physically reasonable assumption that Υ is a Slater determinant. In this case, the required antisymmetry of the wave function is inherent

in our assumptions on Υ and the one dimensional function ψ is symmetric, i.e., the electrons behave like bosons in one dimension.

It is straightforward to show that

$$(2.4) \quad E_0^{\text{conf}}(N, Z, B) = \sqrt{B} \inf_{\|\psi\|=1} \langle h(N, Z, M)\psi, \psi \rangle + NB$$

where have scaled out the field strength B so that

$$(2.5) \quad h(N, Z, M) = \sum_{j=1}^N \left[-\frac{1}{M} \frac{d^2}{dx_j^2} - Z\tilde{V}(x_j) \right] + \sum_{j < k} \tilde{W}(x_j - x_k)$$

and the only remnant of the magnetic field is in the “mass” $M = B^{-1/2}$ and the effective one-dimensional potentials \tilde{V} and \tilde{W} will be defined below for each model.

For the zero model, one easily finds [BR1] that

$$(2.6) \quad \tilde{V}(x) = V_0(x) \quad \text{and} \quad \tilde{W}(u - v) = \frac{1}{\sqrt{2}} V_0 \left(\frac{|u - v|}{\sqrt{2}} \right).$$

Note $V_0(x) \approx \frac{1}{|x|}$ for large $|x|$. Thus, for large separations,

$$(2.7) \quad \tilde{W}(u - v) \approx \frac{1}{\sqrt{2}} \frac{\sqrt{2}}{|u - v|} = \frac{1}{|u - v|}.$$

However, not only is the singularity removed at $u = v$, $\tilde{W}(0)$ is smaller by a factor of $\frac{1}{\sqrt{2}}$ than $\tilde{V}(0)$. This means that if two electrons are simultaneously near the nucleus, the price paid from the electron-electron repulsion is smaller than that gained from the electron-nuclear attraction. Although this effect seems to play an important role in binding additional electrons, it may be partially offset by the price paid in kinetic energy if one attempts to constrain both electrons near the nucleus. See [BR1] for further discussion.

For the Slater model it can be shown [BR2] that

$$(2.8) \quad \tilde{V}(x) \equiv V_{\text{av}}^N(x) = \frac{1}{N} \sum_{m=0}^{N-1} V_m(x) \quad \text{and}$$

$$(2.9) \quad \tilde{W}(u - v) = \frac{1}{\sqrt{2}} \sum_{j=0}^{N-1} c_j V_{2j+1} \left(\frac{|u - v|}{\sqrt{2}} \right)$$

where $c_j > 0 \forall j$ and $\sum_j c_j = 1$ so that the effective interaction is a convex combination of V_m with odd $m = 1, 3, \dots, 2N - 1$, albeit with the same $\frac{1}{\sqrt{2}}$ scaling as in (2.7). Note that the convex sum in (2.9) above includes contributions from V_m with $m > N$. Properties (b) and (d) of Section 4 imply that $V_m(0)$ is decreasing in m . Therefore, one expects a decrease in the electron-electron repulsion \tilde{W} in addition to that from the factor of $\frac{1}{\sqrt{2}}$. However, delicate combinatorics would be needed to verify this exactly.

Some obvious variations on these models are possible and discussed briefly in [BR1, BR2]. It is interesting to note that if $\Upsilon = \prod_{k=1}^N \gamma_m(y_k, z_k)$ with m odd, then the convex sum analogous to (2.9) contains only terms V_{2j} with even subscript.

It is also worth noting that

$$(2.10) \quad \lim_{\beta \rightarrow \infty} \frac{\beta}{\log \beta} V_m(\beta x) = \delta(x)$$

in the sense of tempered distributions. This implies that the potentials \tilde{V} and \tilde{W} which occur in our models have an analogous delta potential behavior as $\beta \rightarrow \infty$. The proof [BD] of (2.10) uses the Fourier transform (property (k) in Section 4) of the potentials $V_m(x)$, particularly the observation that $\hat{V}_m(\xi)$ has a logarithmic singularity at $\xi = 0$. Similar limiting behavior (with $\beta = \sqrt{B}$) was observed by [LSY] for potentials in the three-dimensional Hamiltonian (2.1). It can also be shown [BD] that if (2.5) is appropriately rescaled and the potentials replaced by the corresponding delta potentials, the result is a one-dimensional Hamiltonian whose semi-classical limit (on bosonic wave functions) as $Z \rightarrow \infty$ is precisely that given by the (fermionic) hyperstrong functional in [LSY]. Since their functional was shown to describe the $Z, B/Z^3 \rightarrow \infty$ limit of the three-dimensional Hamiltonian (2.1), this provides additional justification for our models. Even the simple-minded zero model has the correct asymptotic behavior.

3. Maximum Negative Ionization

In the absence of a magnetic field, one expects that the maximum number of electrons a nucleus with charge Z can bind is $N_{\max}(Z) = Z + 1$ or $Z + 2$. However, only the somewhat weaker result of asymptotic neutrality has been proved rigorously [LSST]. If electrons behave like bosons, asymptotic neutrality does not hold and N_{\max} behaves asymptotically roughly like $1.21Z$. (See [Sol] for details and references to earlier work on bosonic atoms.) In [Lb] Lieb gave a simple argument which showed that $N_{\max} < 2Z + 1$, independent of particle statistics. Thus, it may seem somewhat surprising that [LSY] showed that for atoms in extremely strong magnetic fields

$$(3.1) \quad \liminf_{Z, B/Z^3 \rightarrow \infty} \frac{N_{\max}(Z)}{Z} \geq 2.$$

The study of one-dimensional models in [BR1] was initiated, in part, by the hope of proving an asymptotic upper bound of the form $N_{\max} \leq 2Z$ as $B, Z \rightarrow \infty$. Although we did not succeed in proving such a bound, even for our simplified one-dimensional models, we believe that they offer considerable insight into both the reasons for binding an “extra” Z electrons and the reasons why the localization techniques developed to bound N_{\max} fail in the strong field case.

It is generally believed that enhanced binding occurs in strong magnetic fields because the field confines the electrons in two dimensions and effectively reduces the atom to a one-dimensional system. Although there is some truth to this, it was shown in [LSY] that atoms do not become truly one-dimensional unless $B > Z^3$ and the field strength is greater than anything seen on earth. (Sufficiently strong magnetic fields do exist on the surface of neutron stars, making this analysis of some interest in astrophysics.) Moreover, the binding enhancement achieved by making the system effectively one-dimensional can only account for small effects, such as the fact [AHS] that singly negative ions always have infinitely many bound states in a magnetic field. It cannot account for the binding of an additional Z electrons.

The results in [BR1] suggest that the primary mechanism for binding additional electrons in strong fields is the fact that the effective reduction in the strength of the electron-electron repulsion permits two electrons to be near the nucleus simultaneously. However, the one-dimensional confinement also delocalizes the electron. This effect is seen in the Hamiltonian $h(N, Z, B^{-1/2})$ given by (2.5) where the effective mass is $M = B^{-1/2}$ so that in strong fields the electrons behave

like extremely light particles. The uncertainty principle then implies that trial wave functions which localize the electrons cannot yield bound states.

Since Lieb's strategy [**Lb**] for finding an upper bound on $N_{\max}(Z)$ does not require an explicit localization, it might seem well-suited to atoms in strong magnetic fields. However, Lieb's method actually has an implicit localization (which is based on an idea of Benguria [**Ben**] for spherically symmetric atoms) for which the localization error is zero in three dimensions. However, as explained in [**BR1**], the localization error is necessarily non-zero in one-dimension. (This is a consequence of the fact that non-positive potentials always have at least one bound state in one dimension. Thus, the phenomenon of enhanced binding in one dimension actually contributes to the delocalization of the electrons.) Using Lieb's method for the zero model, we were only able to show in [**BR1**] that $N_{\max}(Z, B) < 2Z + 1 + c\sqrt{B}$ for an explicit constant c . In the interesting case $B = O(Z^3)$, this yields a bound of the form $N_{\max} < 2Z + cZ^{3/2}$, rather than a linear one.

Surprisingly, one can get a better bound using the Ruskai-Sigal localization method. (See [**Rusk**] for a summary.) For both the zero model and the Slater model, we can prove the following result.

THEOREM 3.1. *Let $N_{\max}(Z, B)$ be the maximum number of electrons for which the Hamiltonian (2.5) has a bound state, and assume that the potentials \tilde{V} and \tilde{W} have either the form (2.6) corresponding to the zero model or the form (2.8) and (2.9) corresponding to the Slater model. Then for every $\alpha > 0$ and $\beta > 0$ there is a constant $C_{\alpha\beta}$ such that*

$$(3.2) \quad N_{\max}(Z, B) < C_{\alpha\beta} Z^{1+\alpha} B^{\beta}$$

where α, β can be arbitrarily small and, in the case of the Slater model $B \geq Z^{3+\gamma}$ for some $\gamma > 0$.

This result can be improved slightly to

$$(3.3) \quad N_{\max}(Z, B) < C_{\omega} [Z(\log Z)^2 + Z \log Z (\log B)^{1+\omega}]$$

where, as above, $\omega > 0$ can be arbitrarily small and in the case of the Slater model $B \geq Z^{3+\gamma}$. Because the electrons in the one-dimensional model are essentially bosonic, this is the best that one can hope to achieve with the Ruskai-Sigal method.

In the case of the Slater model, the Landau level portion of the wave function Υ is antisymmetric. Hence, the one-dimensional part of the wave function ψ must be symmetric. Even for the zero model, it is physically reasonable to treat the electrons in the one-dimensional model as essentially bosonic. In the Ruskai-Sigal method, the system is divided into a small “inner” ball in which binding is precluded because the electrons are confined to a small region, and an “outer” ball in which the localization error becomes negligible as $Z \rightarrow \infty$. For bosonic systems, one can always squeeze the electrons closer together, yielding a smaller cut-off ρ than for fermions. This feature is the *only* factor which precludes extending the proof of asymptotic neutrality in [**LSST**] to bosonic atoms. This demonstrates that the localization error is not simply a technical artifact, but a reflection of a real physical effect.

For atoms in strong magnetic fields, the cut-off radius ρ is not small. Instead $\rho \sim N\sqrt{B}Z^{-2}(\log \frac{Z^2}{B})^{-2}$ which grows with B . For $B = O(Z^3)$ and $N = O(Z)$, roughly speaking (i.e., ignoring the \log term) $\rho \sim Z^{1/2} \sim B^{1/6}$. Thus, the localization method can be used to obtain a (non-optimal) upper bound on N_{\max}

despite the fact that the electrons are highly delocalized and the size of the “inner” region becomes arbitrarily large as $B \rightarrow \infty$. However, the non-optimal bounds above are probably the best one can expect from configuration space localization. It seems likely that a proof of better upper bounds will require the use of phase space localization techniques.

4. Properties of $V_m(x)$

The functions $V_m(x)$ are even and well-defined for $x > 0$. Although the primary interest in physical applications is for integer $m \geq 0$, it is easy to see from the form (1.3) that they can be extended to complex m with $\Re(m) > -1$. For $\Re(m) > -\frac{1}{2}$ they are also well-defined for $x = 0$. In this note we restrict ourselves to non-negative x and real $m > -1$.

It is convenient to define $V_{-1}(x) = \frac{1}{|x|}$ and note that this is justified in the sense that $\lim_{m \rightarrow -1^+} x^{-1} V_m(x) = 1$ for all $x > 0$.

We now summarize the properties of $V_m(x)$ for $x \in (0, \infty)$. Unless otherwise stated m is real and $m > -1$. For proofs and further discussion, see [RW].

Summary of Properties of $V_m(x)$:

- a) $V_m(x)$ satisfies the inequality $\frac{1}{\sqrt{x^2 + m}} > V_m(x) > \frac{1}{\sqrt{x^2 + m + 1}}$ where the upper bound holds for $m > 0$ and the lower for $m > -1$.
- b) $V_m(x)$ is decreasing in m . In particular, $V_{m+1}(x) < V_m(x) < \frac{1}{x}$.
- c) The expression $mV_m(x)$ is increasing in $m > -1$.
- d) For $m > -1/2$, the definition of $V_m(x)$ can be extended to $x = 0$ and

$$V_m(0) = \frac{\Gamma(m + \frac{1}{2})}{\Gamma(m + 1)}.$$

For integer m , this becomes

$$V_m(0) = \frac{(2m)!}{2^{2m}(m!)^2} \sqrt{\pi} = \frac{1 \cdot 3 \cdot 5 \dots (2m-1)}{2 \cdot 4 \cdot 6 \dots (2m)} \sqrt{\pi}$$

while for large m Stirling’s formula implies

$$V_m(0) \approx \left(\frac{m - \frac{1}{2}}{m}\right)^m \left(\frac{e}{m}\right)^{1/2} \approx \frac{1}{\sqrt{m}}$$

which is consistent with property (a).

- e) For all $m \geq 0$, V_m satisfies the differential equation

$$V'_m(x) = 2x(V_m - V_{m-1}).$$

- f) For each fixed $m \geq 0$, $V_m(x)$ is decreasing in x .
- g) For $a > 0$, the expression $aV_m(ax)$ increases with a . Hence $aV_m(ax) > V(x)$ when $a > 1$ and $aV_m(ax) < V(x)$ when $a < 1$.
- h) $V_0(x)$ is convex in $x > 0$; however, $V_m(x)$ is *not* convex when $m > \frac{1}{2}$.
- i) For integer m , $1/V_m(x)$ is convex in $x > 0$.
- j) For integer m , the ratio $V_{m+1}(x)/V_m(x)$ is increasing in $x > 0$.
- k) The Fourier transform is given by

$$\widehat{V}_m(\xi) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} V_m(x) e^{-ix\xi} dx = \frac{4^{m+1}}{\sqrt{2\pi}} \int_0^{\infty} \frac{s^m e^{-s}}{(|\xi|^2 + 4s)^{m+1}} ds$$

i) For large x , it follows from property (a) that

$$\frac{m}{2(x^2 + m)^{3/2}} \leq \frac{1}{x} - V_m(x) < \frac{m+1}{2x^3}$$

while (1.3) yields the asymptotic expansion

$$V_m(x) = \frac{1}{x} - \frac{m+1}{2x^3} + \frac{3(m+2)(m+1)}{8x^5} + O\left(\frac{1}{x^7}\right).$$

The lower bound in (a) was proved earlier (at least for integer m) by Avron, Herbst and Simon [AHS]. Properties (b) and (c) imply that $V_m(x)$ is decreasing in m , while $mV_m(x)$ is increasing; this gives an indication of the delicate behavior of V_m . The differential equation (e) can be verified using integration by parts in (1.3). Property (f) follows directly from (b) and (e). Property (g) follows from (1.3) and the observation that $\frac{a}{\sqrt{a^2x^2 + u}}$ is increasing in a . It is useful in analyzing $\tilde{W}(u - v)$ since it implies $\frac{1}{\sqrt{2}}V_m\left(\frac{|u-v|}{\sqrt{2}}\right) < V_m(|u-v|)$. Property (h) follows from a straightforward analysis of the differential equation (e) which implies that $V'_m(0) = 0$ for $m > \frac{1}{2}$. In the next section, we will see that the cusp at $x = 0$ and the convexity of $V_m(x)$ in $x > 0$ return when $V_m(x)$ is replaced by $V_{\text{av}}^N(x)$ as in the Slater model.

The convexity of $1/V_m(x)$ can be rewritten as

$$\frac{1}{\frac{1}{2}V_m\left(\frac{x+y}{2}\right)} \leq \frac{1}{V_m(x)} + \frac{1}{V_m(y)}$$

Using property (g) with $a = \frac{1}{2}$, one easily finds that this implies

$$\frac{1}{V_m(x+y)} \leq \frac{1}{V_m(x)} + \frac{1}{V_m(y)}.$$

Since $1/V_m(x) \approx |x|$ for large $|x|$, this subadditivity inequality plays the role of the triangle inequality in applications. The proof of (i) is extremely delicate. Because $1/V_m(x) \approx x$ for large x , we need to prove the convexity of a function that is nearly linear so that its second derivative is extremely close to zero. Proving that this derivative is positive is equivalent to proving some rather sharp inequalities on the ratio $V_m(x)/V_{m-1}(x)$.

In the special case $m = 0$ these inequalities (which are also discussed in [BR1] and [SW]) are equivalent to

$$(4.1) \quad g_\pi(x) \leq V_0(x) < g_4(x)$$

for $x > 0$, where

$$(4.2) \quad g_k(x) = \frac{k}{(k-1)x + \sqrt{x^2 + k}}.$$

Multiplying (4.1) by $x = \frac{1}{V_{-1}(x)}$ converts this to a bound on the ratio $\frac{V_0(x)}{V_{-1}(x)}$. To obtain general ratio bounds, define

$$(4.3) \quad G_k^m(y) = \frac{ky}{(k-1)y - m + \sqrt{(y+m)^2 + ky}}.$$

Then it is shown in [RW] that

$$(4.4) \quad G_8^{m-1}(x^2) < \frac{V_m(x)}{V_{m-1}(x)} < G_4^m(x^2)$$

for all integer $m \geq 0$ and $x > 0$. The sense in which these bounds are optimal is discussed in [RW]. Our proof of these inequalities relies on an inductive argument and, hence, is valid only for integer m . A proof extending them to general real $m > -1$ would immediately imply that properties (i) and (j) also hold for general real $m > -1$.

Another interesting open question is whether or not $V_m(x)$ is convex in m ? In particular, is $2V_m(x) \leq V_{m+1}(x) + V_{m-1}(x)$? It follows from property (e) that this is equivalent to asking if $V'_m(x)$ is increasing in m .

5. Recursion and Averaged Potentials

Using integration by parts on (1.3) one easily finds that V_m satisfies the recursion relation

$$(5.1) \quad V_m(x) = \frac{1}{m} [(m - \frac{1}{2} - x^2)V_{m-1}(x) + x^2V_{m-2}(x)].$$

for all $m \in \mathbf{R}$, $m \geq 1$. Iterating this, one finds that when m is a positive integer

$$(5.2) \quad V_m(x) = \frac{1}{2m} \left[(1 - 2x^2)V_{m-1}(x) + \sum_{k=0}^{m-2} V_k(x) + 2|x| \right].$$

These relations are useful for studying $V_{\text{av}}^N(x)$. For example, it follows immediately from (5.2) that

$$(5.3) \quad V_{\text{av}}^N(x) = 2V_N(x) - \frac{2x^2}{N} [V_{-1}(x) - V_{N-1}(x)].$$

This can then be used to show that $V_{\text{av}}^N(x)$ is convex for all $x > 0$. Furthermore $\lim_{x \rightarrow 0^+} \frac{d}{dx} V_{\text{av}}^N(x) = -\frac{2}{N}$, verifying that $V_{\text{av}}^N(x)$ has a cusp at $x = 0$.

It is interesting to note that (5.2) also implies that there are polynomials $P_m(y)$ and $Q_m(y)$ of degree m such that for integer $m \geq 1$

$$(5.4) \quad V_m(x) = P_m(x^2)V_0(x) + xQ_{m-1}(x^2).$$

These polynomials have many interesting properties. In [RW] it is shown that

$$(5.5) \quad P_m(y) = \frac{1}{m} \frac{B(m, \frac{1}{2})}{B(m, \frac{1}{2})} e^{-y} {}_1F_1(\frac{1}{2}, \frac{1}{2} - m, y)$$

where $B(m, n)$ denotes the beta function and ${}_1F_1(\alpha, \gamma, y)$ denotes the indicated confluent hypergeometric function.

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